

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF042722\
 Data File : BF127943.D
 Acq On : 27 Apr 2022 14:07
 Operator : CG\JU
 Sample : N2481-08
 Misc :
 ALS Vial : 7 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 MW-8R

Integration Parameters: rteint.p

Integrator: RTE

Smoothing : ON

Filtering: 5

Sampling : 1

Min Area: 3 % of largest Peak

Start Thrs: 0.2

Max Peaks: 100

Stop Thrs : 0

Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >

Peak separation: 5

Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF042222.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF127943.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.257	330	335	347	rBV	53484	74149	1.94%	0.355%
2	4.463	367	370	377	rVB	35315	40410	1.06%	0.193%
3	5.157	484	488	501	rBV2	47807	73563	1.92%	0.352%
4	5.551	550	555	558	rBV	1795043	1594539	41.64%	7.634%
5	6.545	720	724	733	rBV	1027399	1033053	26.98%	4.946%
6	6.757	758	760	770	rVB2	31885	54237	1.42%	0.260%
7	6.857	773	777	786	rBV2	32502	66113	1.73%	0.317%
8	6.928	786	789	793	rBV	711967	642216	16.77%	3.075%
9	7.057	797	811	812	rBV2	64374	164081	4.28%	0.786%
10	7.498	877	886	889	rBV	2321866	2358603	61.59%	11.292%
11	8.169	992	1000	1004	rBV5	20143	48071	1.26%	0.230%
12	8.216	1004	1008	1011	rBV	929796	843548	22.03%	4.039%
13	8.445	1036	1047	1053	rBV4	18628	62739	1.64%	0.300%
14	9.239	1172	1182	1184	rBV4	39208	107971	2.82%	0.517%
15	9.292	1186	1191	1194	rBV	4095673	3829311	100.00%	18.333%
16	9.392	1204	1208	1226	rVB	2338482	2486469	64.93%	11.904%
17	9.975	1300	1307	1310	rBV	979364	905275	23.64%	4.334%
18	10.345	1367	1370	1373	rBV	138188	103034	2.69%	0.493%
19	10.381	1373	1376	1380	rVB	110784	95190	2.49%	0.456%
20	10.675	1422	1426	1428	rBV	93871	87481	2.28%	0.419%
21	10.763	1437	1441	1447	rBV	1798584	1571885	41.05%	7.526%
22	11.463	1556	1560	1564	rBV	931834	764206	19.96%	3.659%
23	11.839	1621	1624	1627	rVB	87609	69186	1.81%	0.331%
24	12.757	1777	1780	1786	rBV2	46114	74231	1.94%	0.355%
25	13.051	1826	1830	1833	rBV	2793024	2435014	63.59%	11.658%
26	14.110	2006	2010	2014	rBV	628309	558950	14.60%	2.676%
27	15.621	2261	2267	2273	rBV	574895	743606	19.42%	3.560%

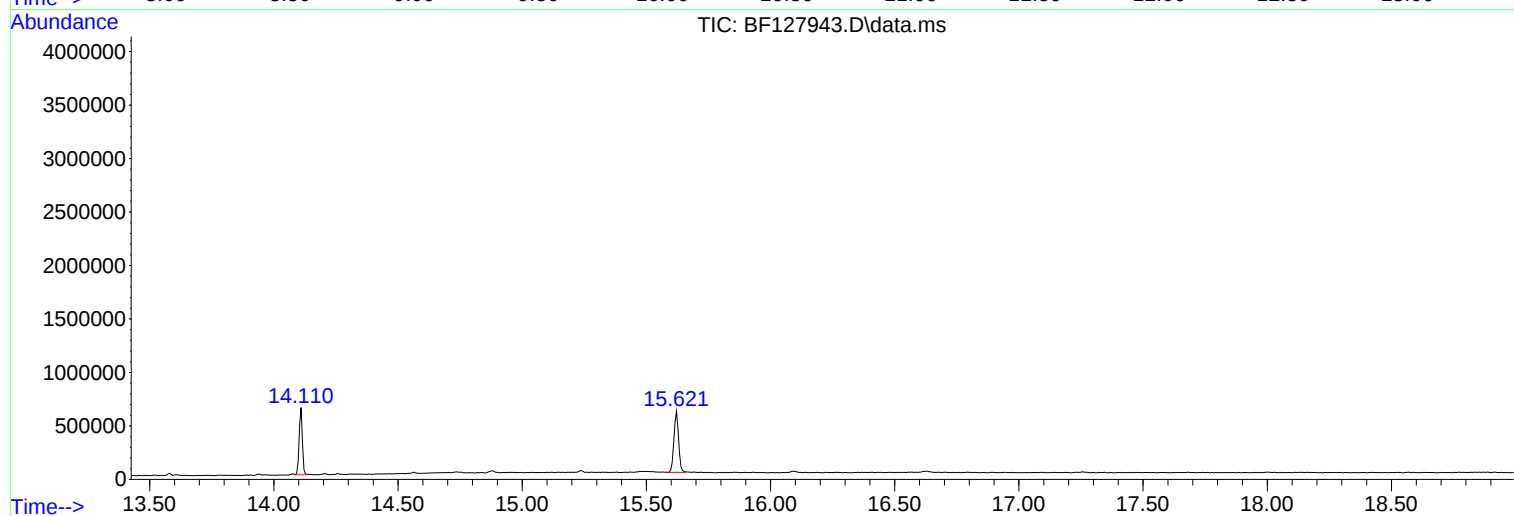
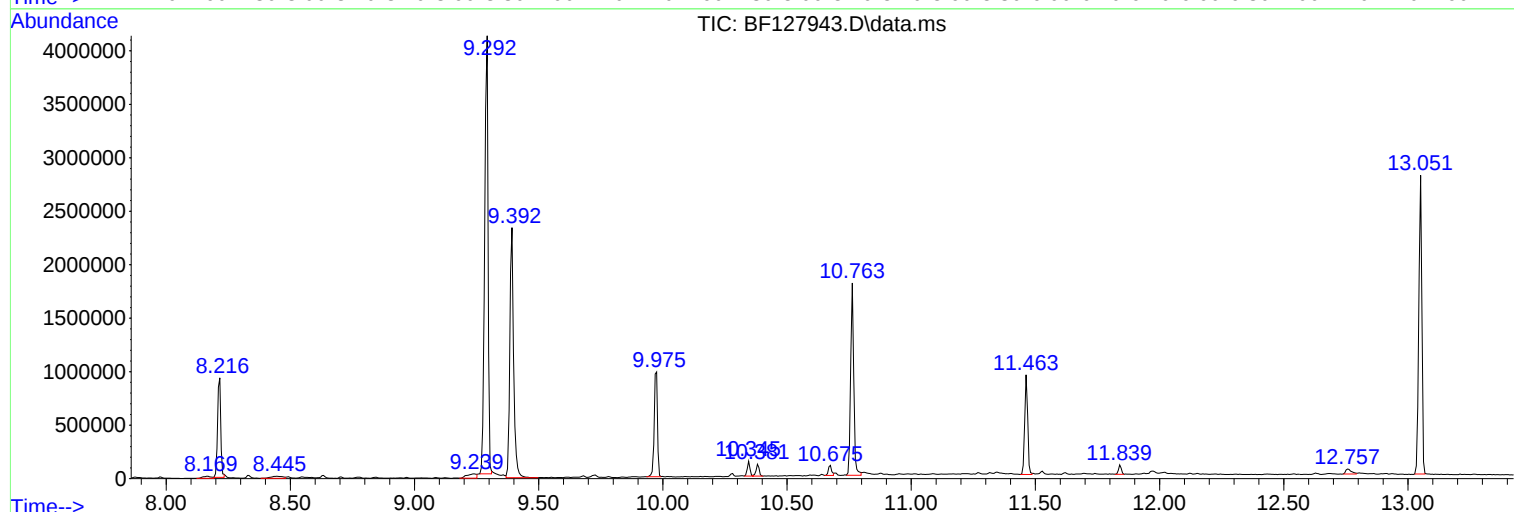
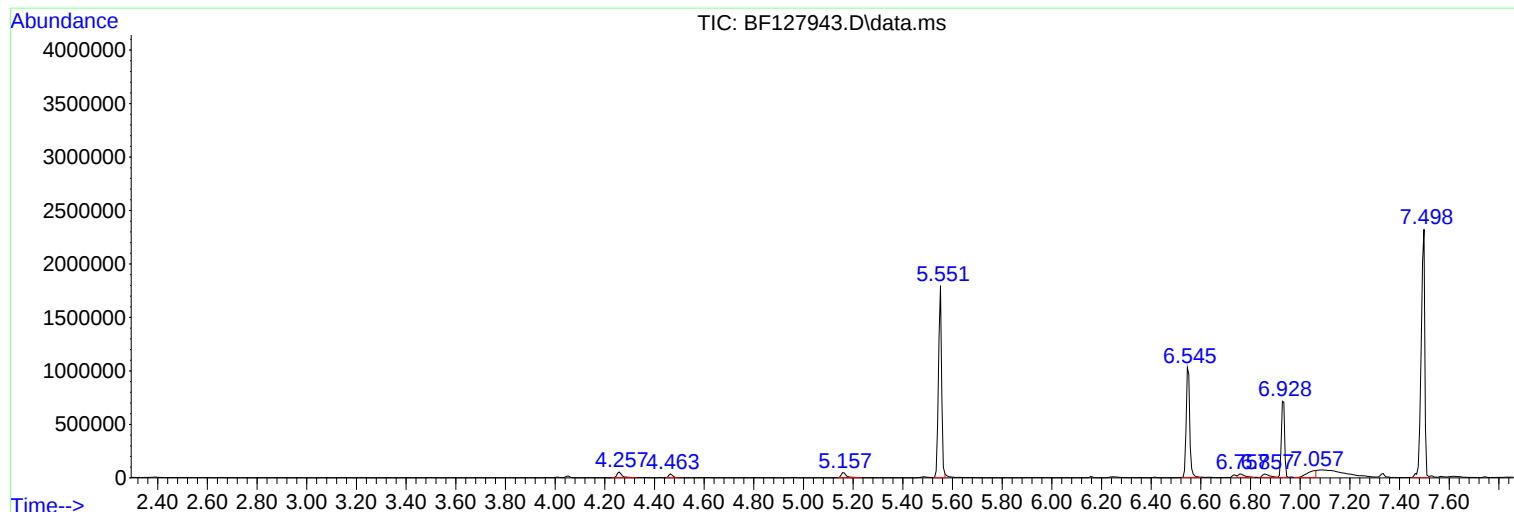
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ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF042222.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P



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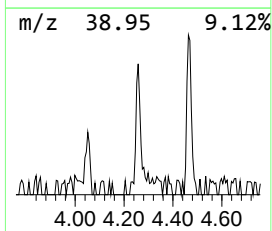
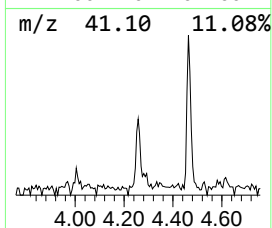
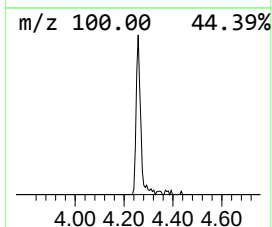
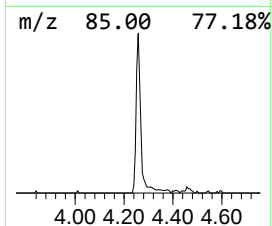
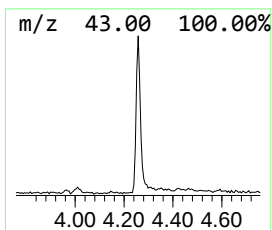
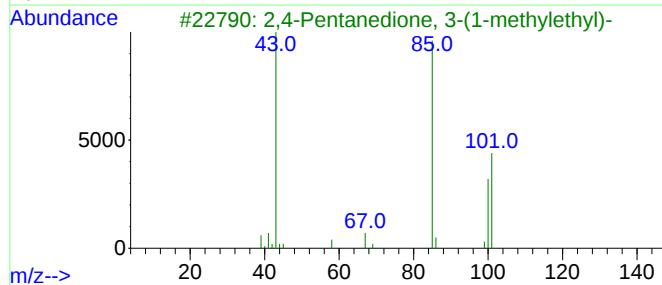
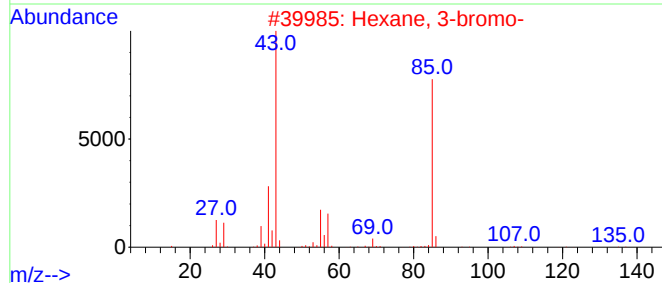
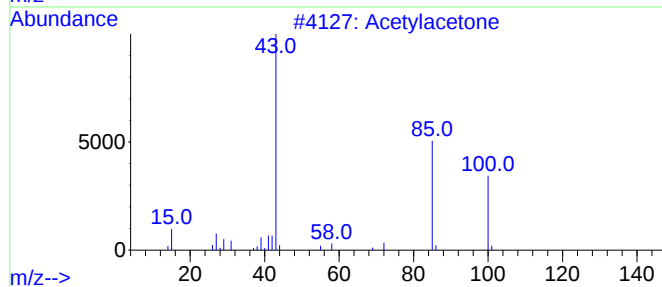
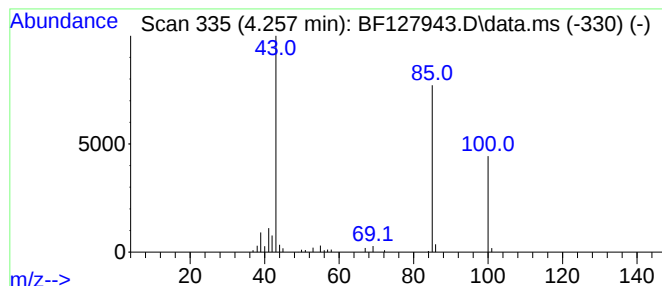
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 Acetylacetone Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.257	2.31 ng	74149	1,4-Dichlorobenzene-d4	6.934

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Acetylacetone	100	C5H8O2	000123-54-6	78
2			Hexane, 3-bromo-	164	C6H13Br	003377-87-5	42
3			2,4-Pentanedione, 3-(1-methyleth...	142	C8H14O2	001540-38-1	42
4			Hexane, 2-bromo-	164	C6H13Br	003377-86-4	42
5			Tetrahydrofuran, 2,2-dimethyl-	100	C6H12O	001003-17-4	36



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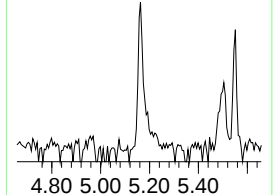
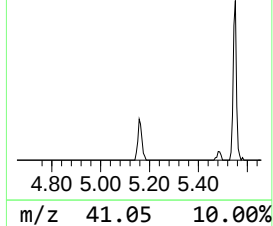
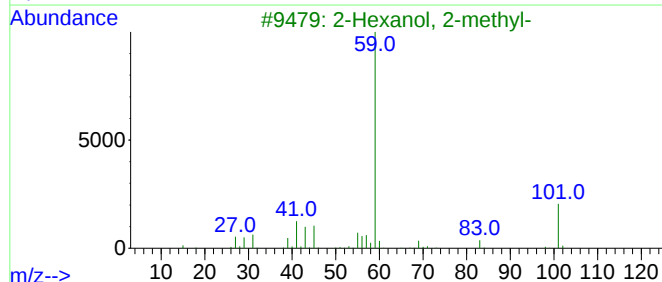
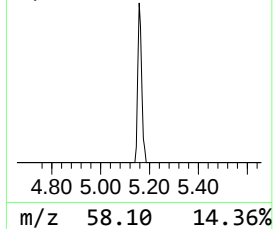
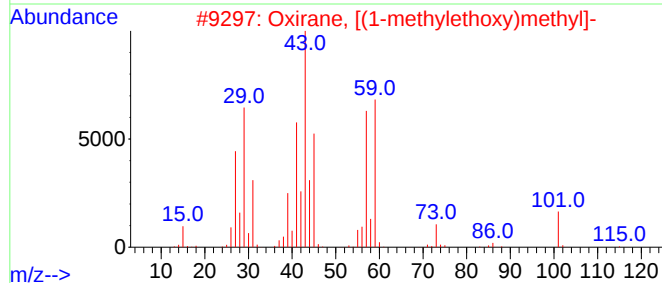
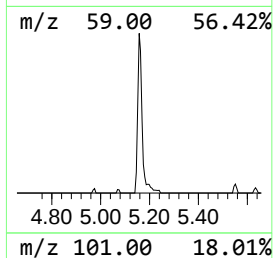
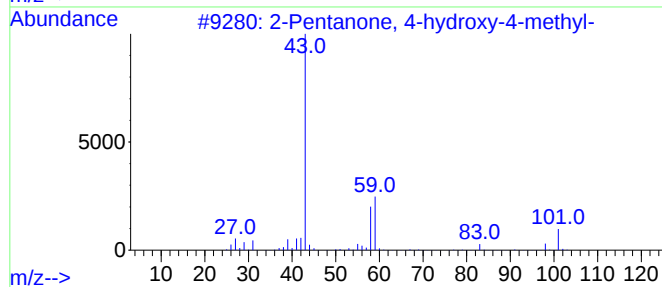
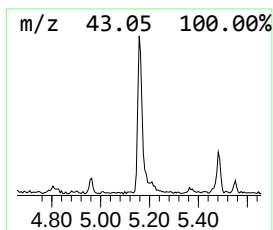
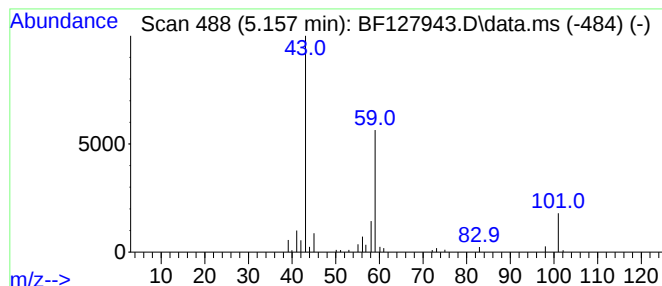
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TIC Integration Parameters: LSCINT.P

Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD			R.T.
5.157	2.29 ng	73563	1,4-Dichlorobenzene-d4			6.934

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59	
2	Oxirane, [(1-methylethoxy)methyl]-	116	C6H12O2	004016-14-2	38	
3	2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	38	
4	n-Propyl t-butyl ether	116	C7H16O	1000334-81-9	33	
5	Cycloserine	102	C3H6N2O2	000068-41-7	33	



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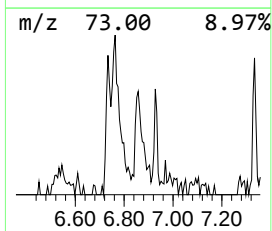
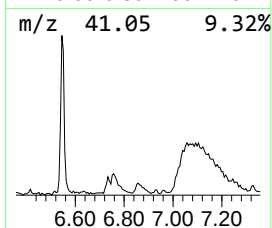
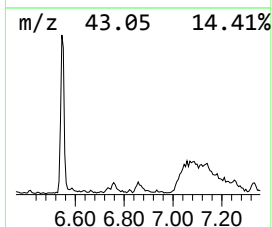
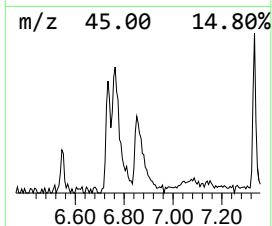
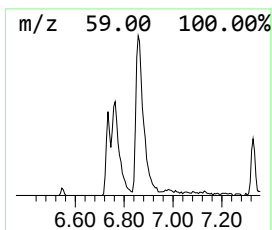
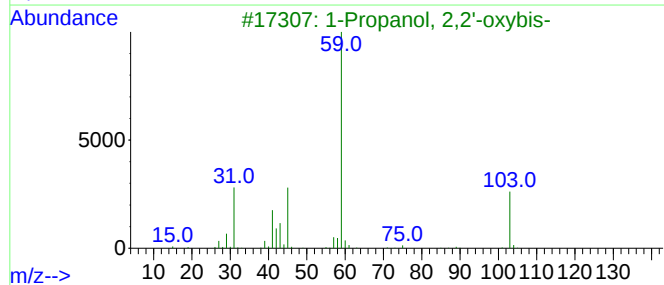
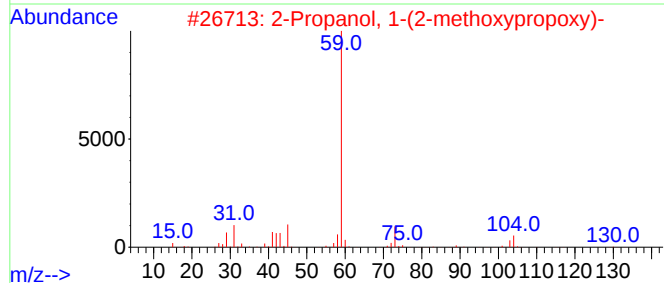
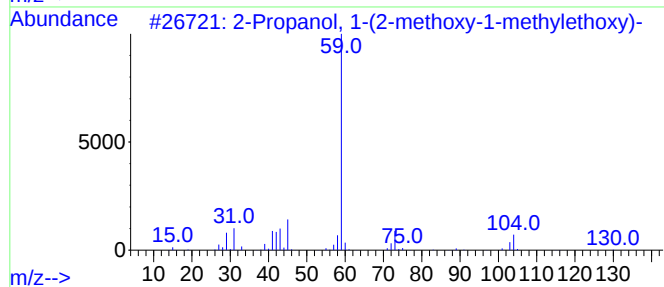
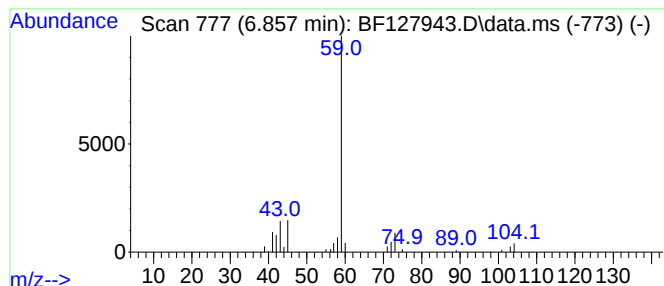
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 2-Propanol, 1-(2-methoxy-1-... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.857	2.06 ng	66113	1,4-Dichlorobenzene-d4	6.934

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Propanol, 1-(2-methoxy-1-methy...	148	C7H16O3	020324-32-7	83		
2	2-Propanol, 1-(2-methoxypropoxy)-	148	C7H16O3	013429-07-7	78		
3	1-Propanol, 2,2'-oxybis-	134	C6H14O3	000108-61-2	72		
4	Dipropylene glycol (isomer 3)	134	C6H14O3	1000506-25-5	72		
5	2-Propanol, 1-[1-methyl-2-(2-pro...	174	C9H18O3	055956-25-7	64		



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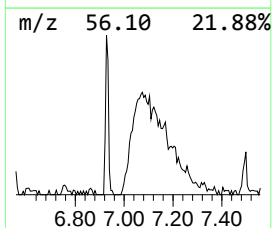
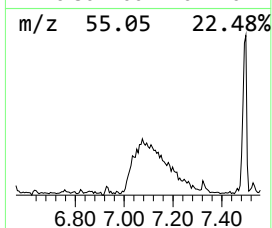
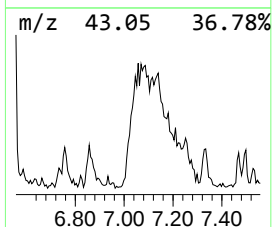
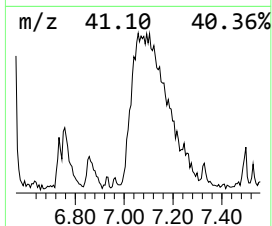
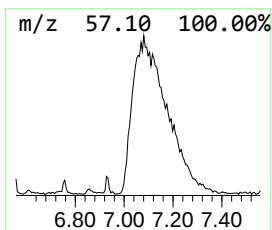
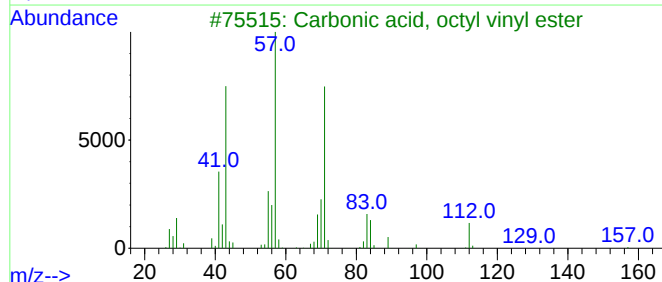
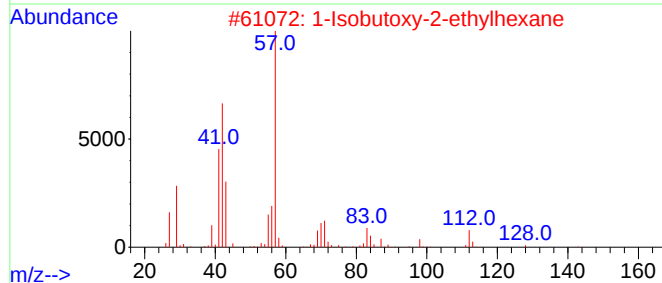
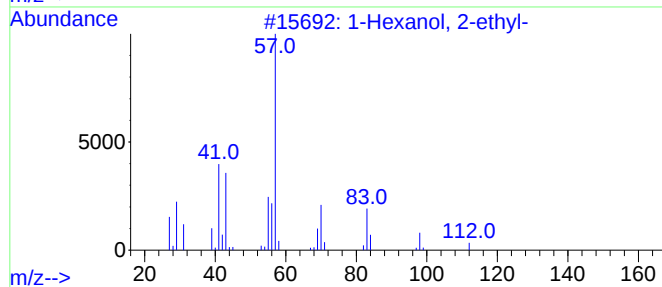
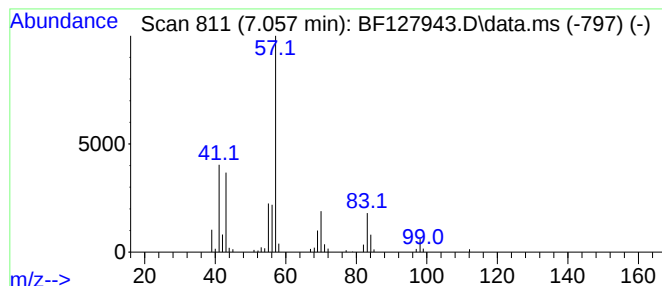
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Peak Number 4 1-Hexanol, 2-ethyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.057	5.11 ng	164081	1,4-Dichlorobenzene-d4	6.934

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	90
2			1-Isobutoxy-2-ethylhexane	186	C12H26O	1000139-90-3	64
3			Carbonic acid, octyl vinyl ester	200	C11H20O3	1000383-25-5	59
4			Carbonic acid, heptyl prop-1-en-...	200	C11H20O3	1000382-54-1	59
5			1-Pentanol, 2-ethyl-4-methyl-	130	C8H18O	000106-67-2	56



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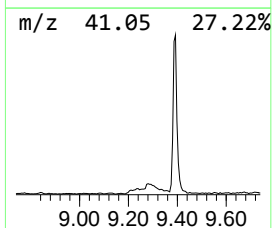
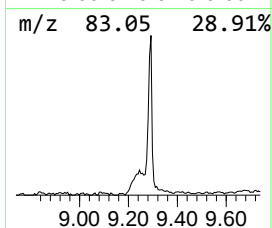
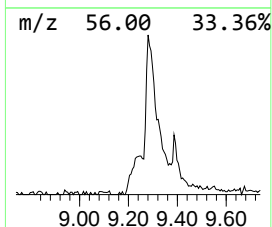
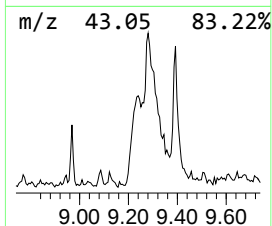
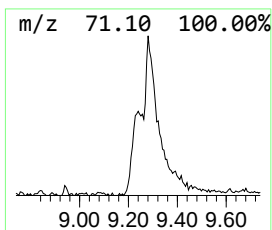
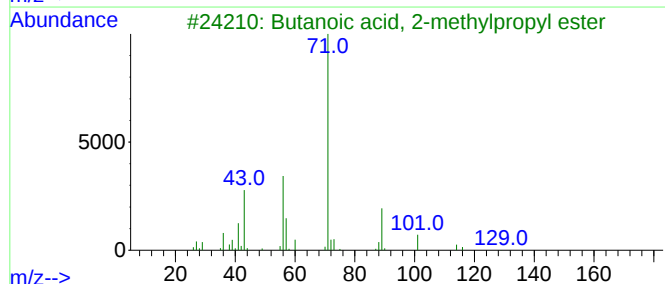
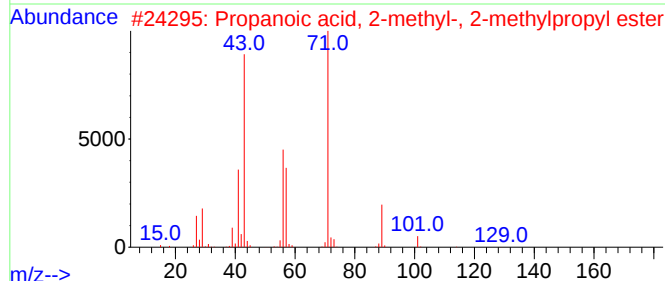
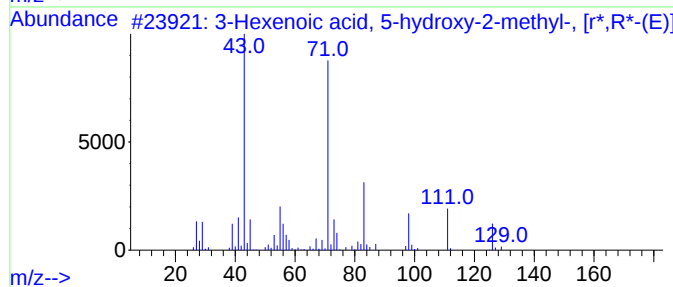
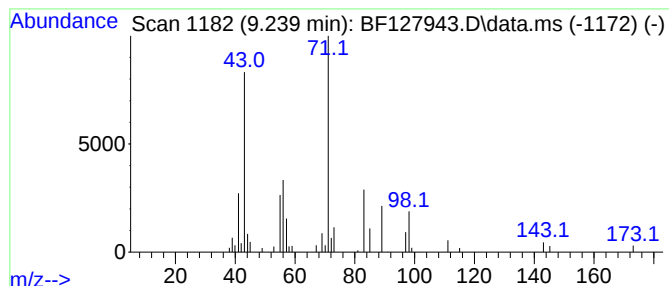
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Peak Number 5 unknown9.239 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.239	2.39 ng	107971	Acenaphthene-d10	9.975

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			3-Hexenoic acid, 5-hydroxy-2-met...	144	C7H12O3	110678-36-9	42
2			Propanoic acid, 2-methyl-, 2-met...	144	C8H16O2	000097-85-8	40
3			Butanoic acid, 2-methylpropyl ester	144	C8H16O2	000539-90-2	40
4			Diethylmalonic acid, heptyl tetr...	342	C19H34O5	1000370-64-2	38
5			2,2,4-Trimethyl-1,3-pentanediol ...	286	C16H30O4	006846-50-0	37



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MW-8R

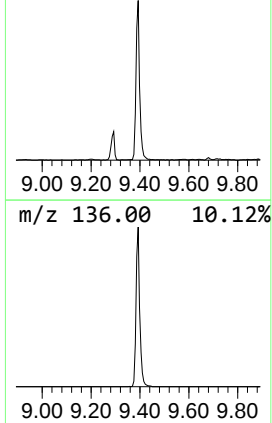
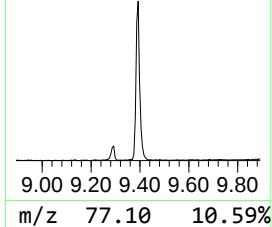
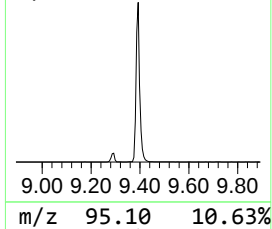
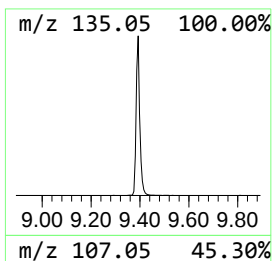
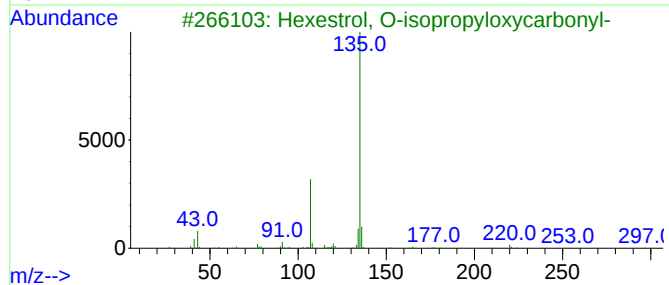
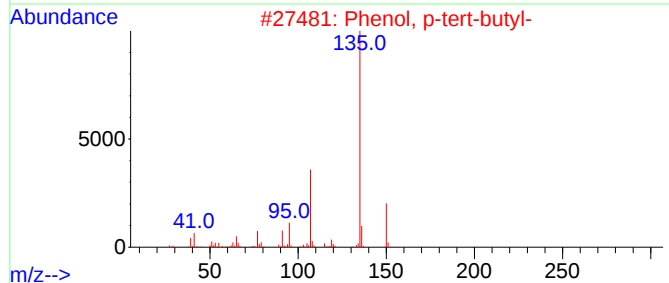
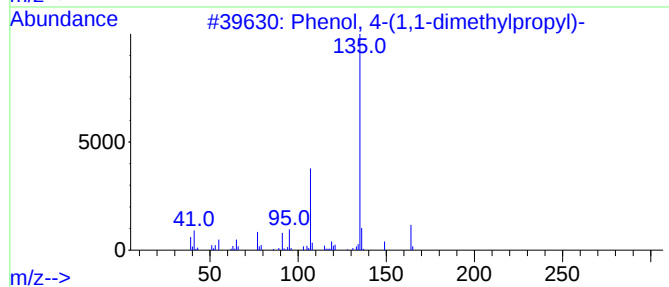
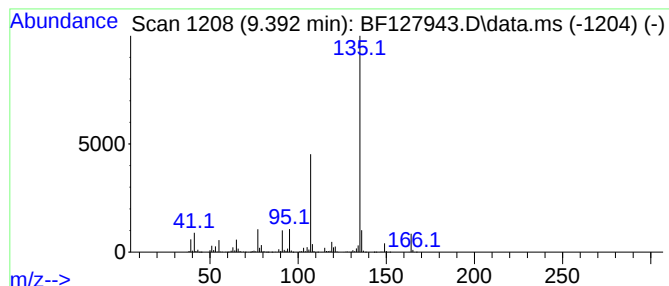
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 Phenol, 4-(1,1-dimethylprop... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.392	54.93 ng	2486470	Acenaphthene-d10	9.975

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Phenol, 4-(1,1-dimethylpropyl)-	164	C11H16O	000080-46-6	93
2			Phenol, p-tert-butyl-	150	C10H14O	000098-54-4	90
3			Hexestrol, O-isopropoxyloxy carbonyl-	356	C22H28O4	1000487-68-4	64
4			4,4'-(1,2-diethylethylene)diphenol	270	C18H22O2	005635-50-7	64
5			Phenol, m-tert-butyl-	150	C10H14O	000585-34-2	64



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF042722\
Data File : BF127943.D
Acq On : 27 Apr 2022 14:07
Operator : CG\JU
Sample : N2481-08
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MW-8R

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF042222.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST0.L
TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Acetylacetone	4.257	2.3	ng	74149	1	6.934	642216	20.0
2-Pentanone, 4-...	5.157	2.3	ng	73563	1	6.934	642216	20.0
2-Propanol, 1-(...	6.857	2.1	ng	66113	1	6.934	642216	20.0
1-Hexanol, 2-et...	7.057	5.1	ng	164081	1	6.934	642216	20.0
unknown9.239	9.239	2.4	ng	107971	3	9.975	905275	20.0
Phenol, 4-(1,1-...	9.392	54.9	ng	2486470	3	9.975	905275	20.0